Radiative transfer model and retrieval algorithm for CLARREO hyperspectral sensor

Xu Liu

B. Wielicki, D. F. Young, M. G. Mlynczak, H. Li, W. Wu, Z. Jin, S. Kato, F. Rose, P. Yang[1], W. Godoy, D. K. Zhou, A. M. Larar, W. L. Smith[2], D. P. Kratz, C. Lukashin, D. G. Johnson, and R. R. Baize, N. Phojanamongkolkij, Brian Soden[3]

NASA Langley Research Center
1. Texas A & M University
2. University of Hampton and University of Wisconsin
3. University of Miami

Presentation outline

- Overview of different radiative transfer models
- Description of the Principal Component-based Radiative Transfer Model (PCRTM)
  - Why PCRTM and how does it work?
  - PCRTM for CLARREO IR: 0.1, 0.25, 0.5, 1.0, 2.0 cm^{-1}
  - PCRTM for RS: 1 cm^{-1} spectral resolution
  - Examples of PCRTM application for CLARREO and other sensors
  - Retrieving atmospheric changes from hyperspectral data using PCRTM
- Summary and Conclusions

Overview of Different Fast RT Models

- **Difficult to model channel radiances or reflectance:**

$$R_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu - \nu^{'}) R(\nu) d\nu' , \quad r_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu - \nu^{'}) r(\nu) d\nu'$$

- LBL calculation of monochromatic layer transmittances or TOA radiances is very time consuming
  - Million mono RT calculations needed
- Convolving monochromatic radiances with Sensor Response Function (SRF) is also time consuming
  - Better to do that in the fast RT model
- The Beer's Law is no longer valid after convolving with SRF:
  - It's difficult to handle inhomogeneous path and multiple gases

$$\int_{\Delta\nu} \phi(\nu) T_{gas1} T_{gas2} d\Delta\nu' \neq \int_{\Delta\nu} \phi(\nu) T_{gas1} d\Delta\nu' \int_{\Delta\nu} \phi(\nu) T_{gas2} d\Delta\nu'$$

$$\int_{\Delta\nu} \phi(\nu) T_{layer1} T_{layer2} d\Delta\nu' \neq \int_{\Delta\nu} \phi(\nu) T_{layer1} d\Delta\nu' \int_{\Delta\nu} \phi(\nu) T_{layer2} d\Delta\nu'$$

Overview of Different Fast RT Models

- Correlated-K Distribution (CKD)
  - Take advantage of the fact that the integrated T or R do not depend on the order of monochromatic frequencies
  - Re-order the monochromatic transmittance (g-ν mapping)
    - Remove redundant information
    - Channel transmittance is a linear combination of a few monochromatic T
      - Weights obtained by quadrature of the smooth g function
  - Only approximate when extending to multiple layers with overlapping molecular absorptions

$$T_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu - \nu')T(\nu)d\nu' = \sum_{i}^{N} w_i T_{\nu_i} + \varepsilon$$

- Exponential Sum Fitting of Transmittance (ESFT)
  - w_i and the spectral location of T_i obtained by a selection/regression process
  - Same shortcoming as CKD
  - A lot of research effort on improving overlapping gases and inhomogeneous atmosphere in the past few decades

Overview of Different Fast RT Models

- Fast Transmittance Models
  - Effective transmittance is a non-linear function of atmospheric parameters

$$k_{\Delta\nu}^{Eff}(l) = -\ln \frac{\int_{\Delta\nu} \Phi(\nu-\nu')T(\nu,l)d\nu'}{\int_{\Delta\nu} \Phi(\nu-\nu')T(\nu,l-1)d\nu'} = f\left[\sec\Theta, T_r, T_z(P,T_r).....\right]$$

  - It has been widely used by various satellite sensors
  - The effective optical depth at a particular layer depends on the properties above that layer
    - Polychromatic RT used
    - Hard to change observation altitude
  - Model depends on training
    - Non-physical parameterization
- Optimal Spectral Sampling (OSS)
  - approximates channel radiances (or transmittances) according to:

$$R_{\Delta\nu}(\nu) = \int_{\Delta\nu} \Phi(\nu-\nu')R(\nu\ )d\nu' = \sum_i w_i R_{\nu_i}$$

  - Similar to frequency sampling method or radiance sampling method
  - Spectral locations/weighting coefficients are obtained through a selection/regression process similar to ESFT
  - RT is done monochromatically
  - Physical parameterization and accurate

Description of Principal Component based Radiative Transfer Model (PCRTM)

- Calculates channel radiances (or transmittances) by linearly combine a set of pre-stored EOF:

$$\vec{R}^{ch} = \sum_{i=1}^{N_{EOF}} c_i \vec{U}_i + \vec{\varepsilon} = \sum_{i=1}^{N_{EOF}} \left(\sum_{j=1}^{N_{mono}} a_j R_j^{mono} \right) \vec{U}_i + \vec{\varepsilon}$$

- EOFs are obtained by performing a Principal Component Analysis (PCA) of channel radiances under a wide range of atmospheric and observation conditions
  - Only dozens to hundreds EOFs needed
- Coefficient C_i are predicted from a few monochromatic radiances
  - The relationship is derived from the properties of eigenvectors and SRF
  - C_i can be treated as super channels which contain all the essential information on a spectrum
- Treats the whole spectra as a whole
  - No need to perform redundant calculations
  - Only a few hundred monochromatic calculations are needed
  - Faster than channel-based RT models
  - Physical parameterization and accurate relative to LBL
- Channel radiance can be calculated by a simple EOF transformation
- Jacobian can be calculated analytically

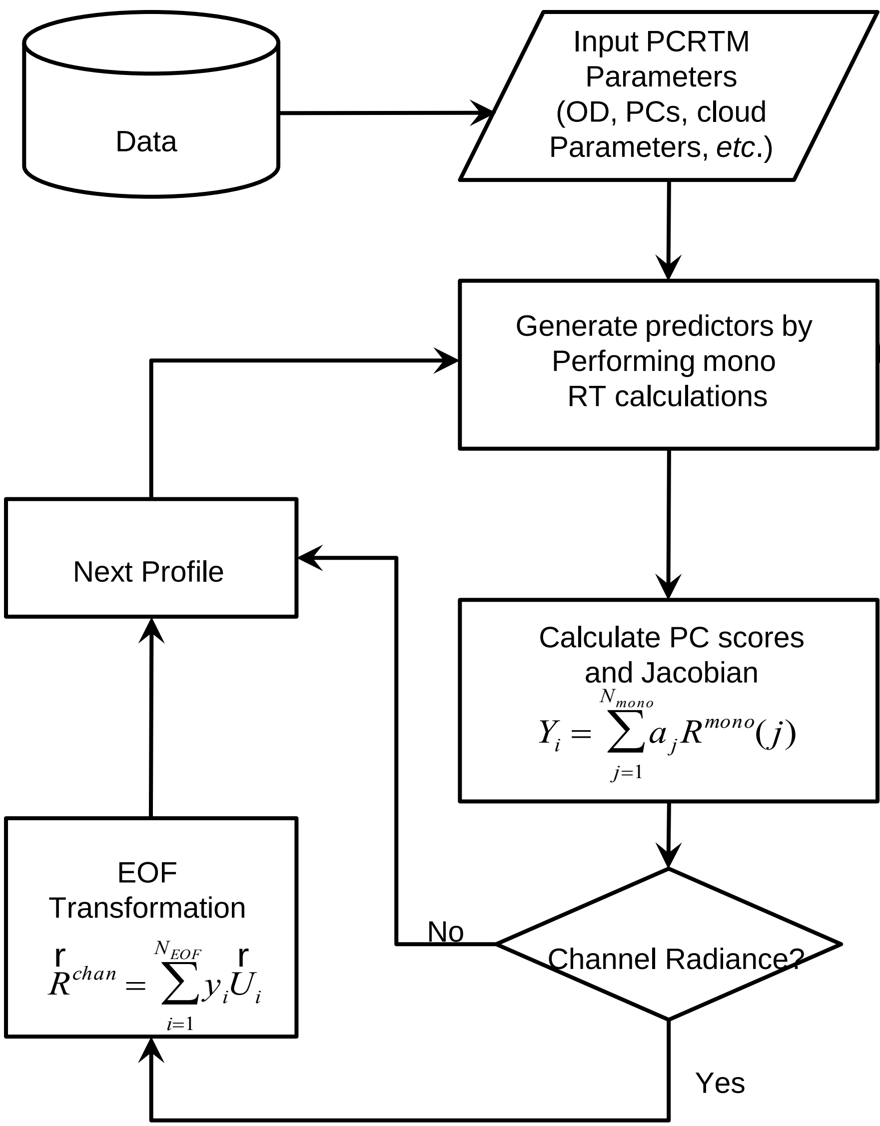
Why PCRTM ?

- Channel-based fast radiative transfer models may be too slow for large data volume
  - Take long time to simulate instantaneous CLARREO spectra for OSSE study
- Hyperspectral data are spectrally correlated
  - Only the first ~50-100 leading eigenvectors are used for optimal fingerprinting
  - Leading EOFs captures all essential information of thousands of channels
  - PCA has been used to reduce instrument noise and to compress spectra
- PCRTM parameterization is physical-based fast model
  - Channel-to-channel spectral correlations are captured by eigenvectors
  - Reduce dimensionality of original spectrum by a factor of 10-90
  - Radiative transfer done monochromatically at very few frequencies
  - Very accurate relative to line-by-line (LBL) RT model (< 0.05K or 0.05%)
  - 3-4 orders of magnitude faster than LBL RT models
  - A factor of 2-100 times faster than channel-based RT models
  - Provide radiative kernel needed for retrievals and climate studies

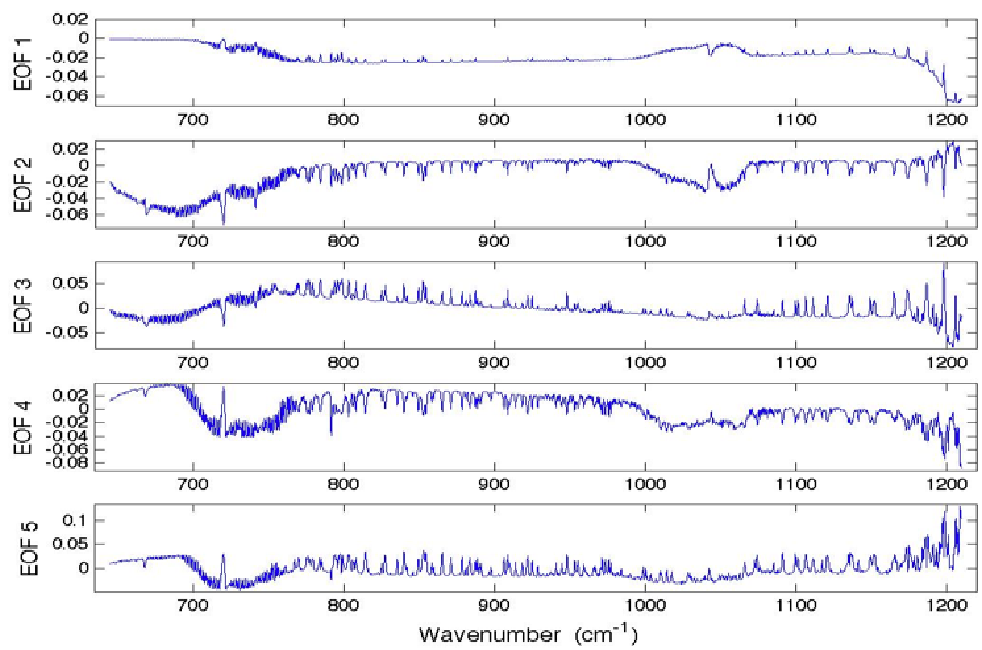
NAST-I Spectral Band	Number of Channels	No. of RT Calc. for All NAST Channels	Predictors per Channel
PCRTM	8632	310-900	0.04-0.1
PFAST	8632	8632	~40
OSS	8632	22316	2.59

How does PCRTM work?

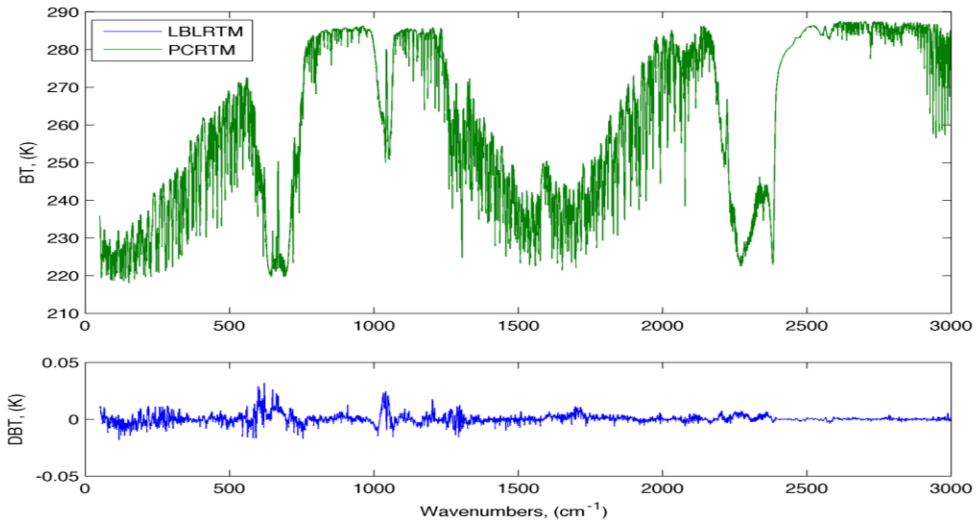
Flow diagram of the PCRTM forward model

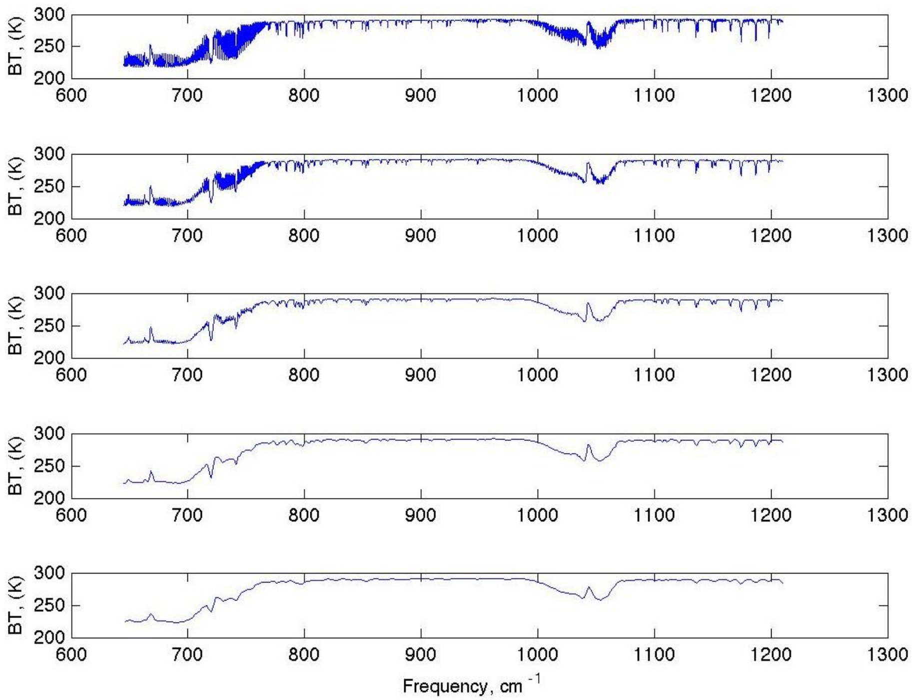


- Monochromatic RT assures Beer's law apply
- RT needs to be done at minimum number of frequencies
  - Orders of magnitude smaller than LBL

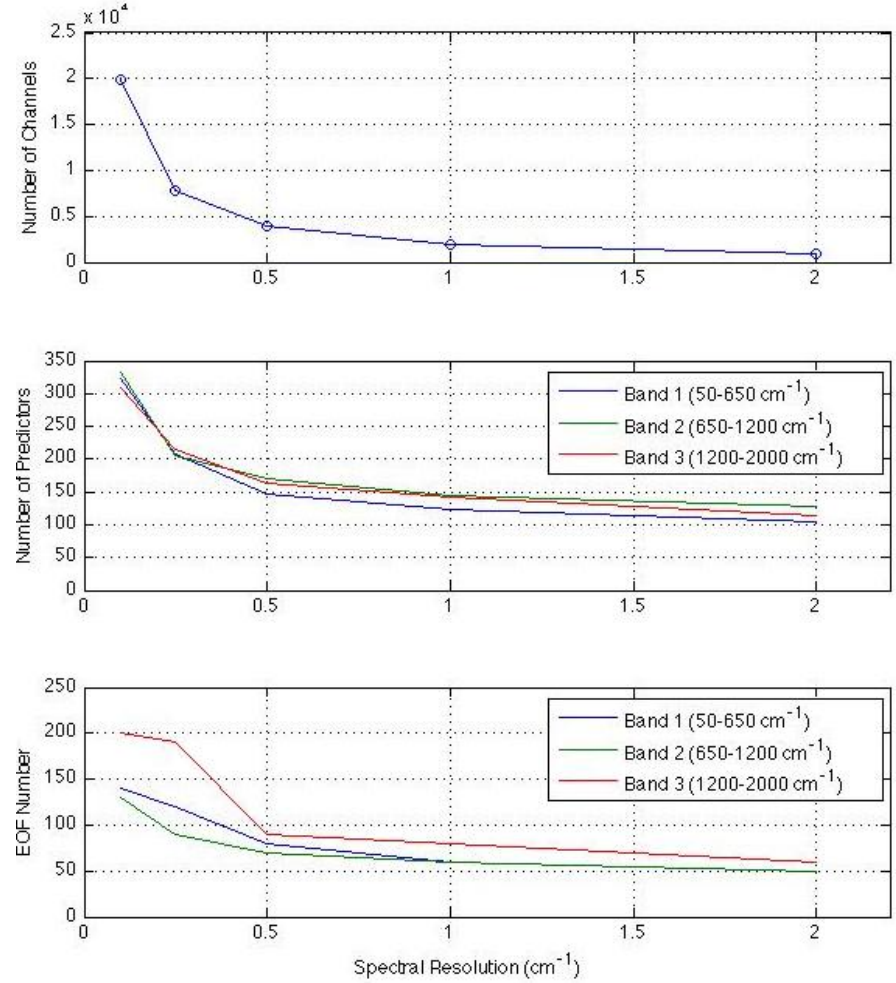


Training of CLARREO PCRTM in IR



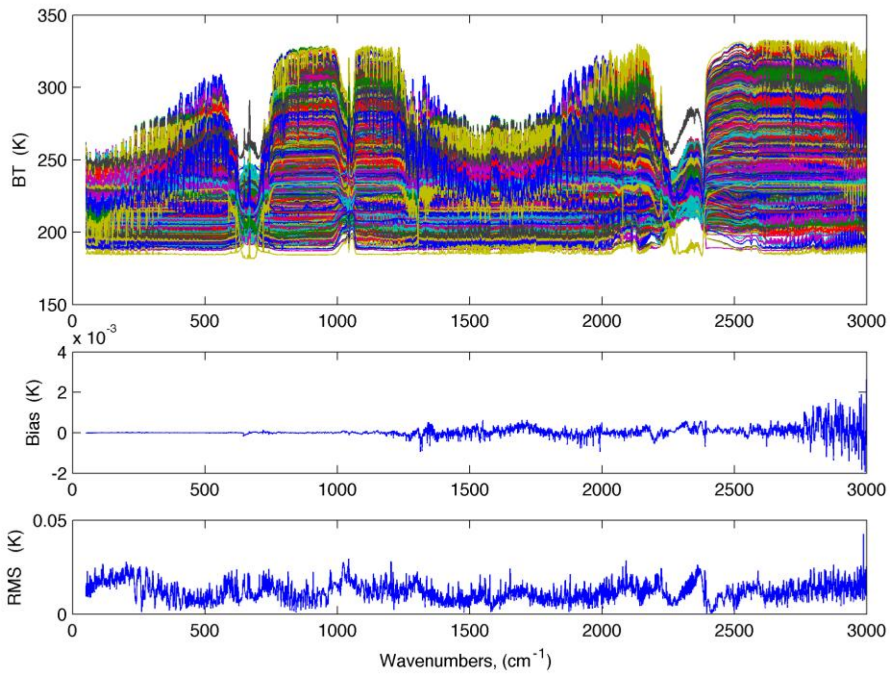


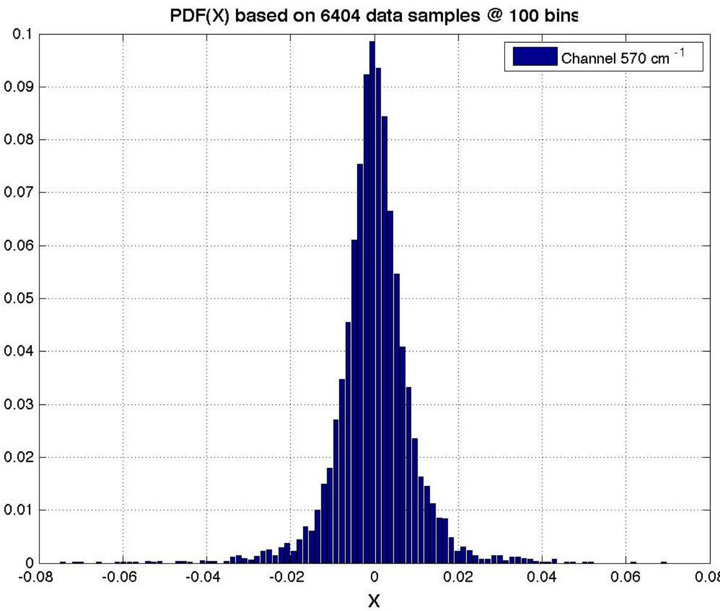
- 0.1 cm^{-1}, 0.25 cm^{-1}, 0.5 cm^{-1}, 1.0 cm^{-1}, and 2.0 cm^{-1}
- 0.1 cm^{-1} model can be used to generate lower spectral resolution instrument forward models
- Reduce >1 million mono RT to < 1000
- EOF and mono numbers decrease with resolution

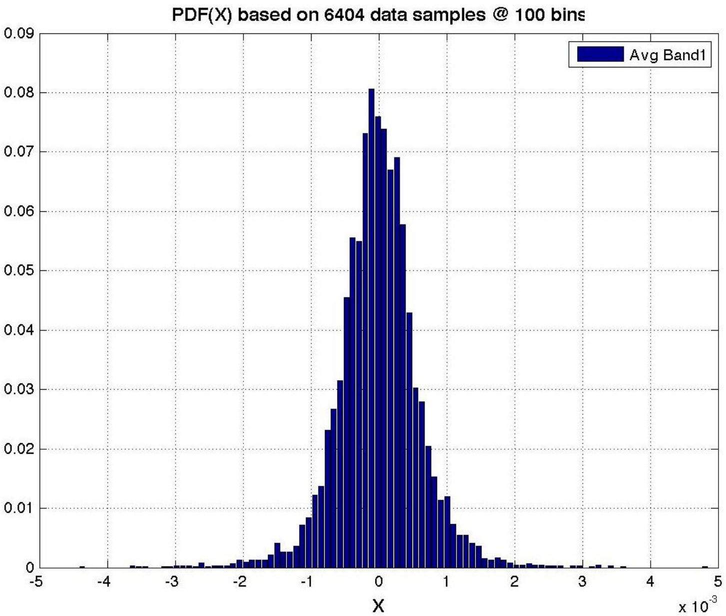


Typical accuracy of the forward model (< 0.03 K relative to LBL)

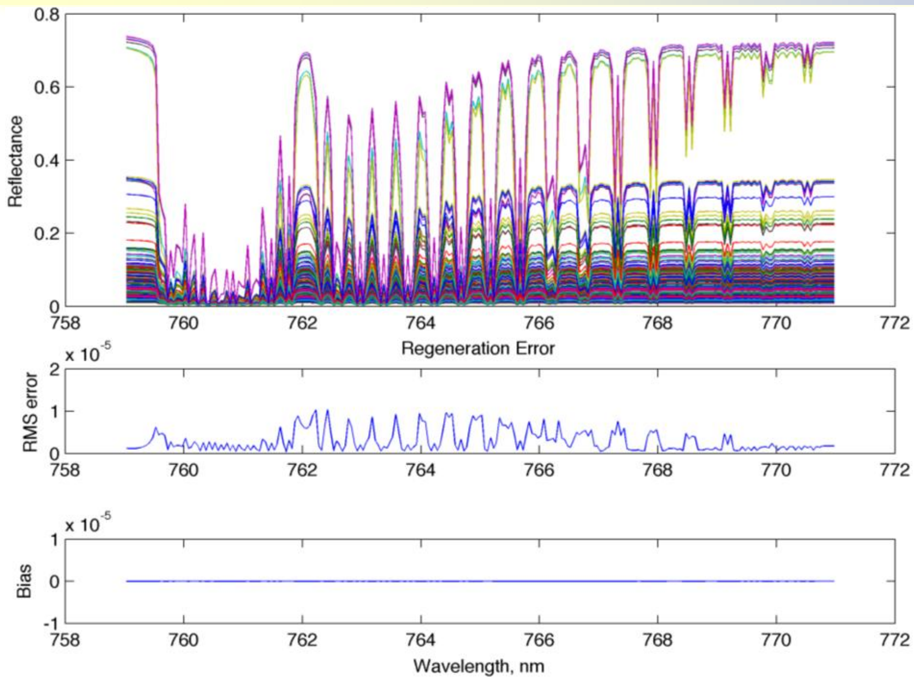
- Bias error relative to LBL is typically less than 0.002
- The PDF of errors at different frequencies are Gaussian distribution
- RMS error less than 0.03K
- Large ensemble of spectra used in the training
- Independent validations perform well

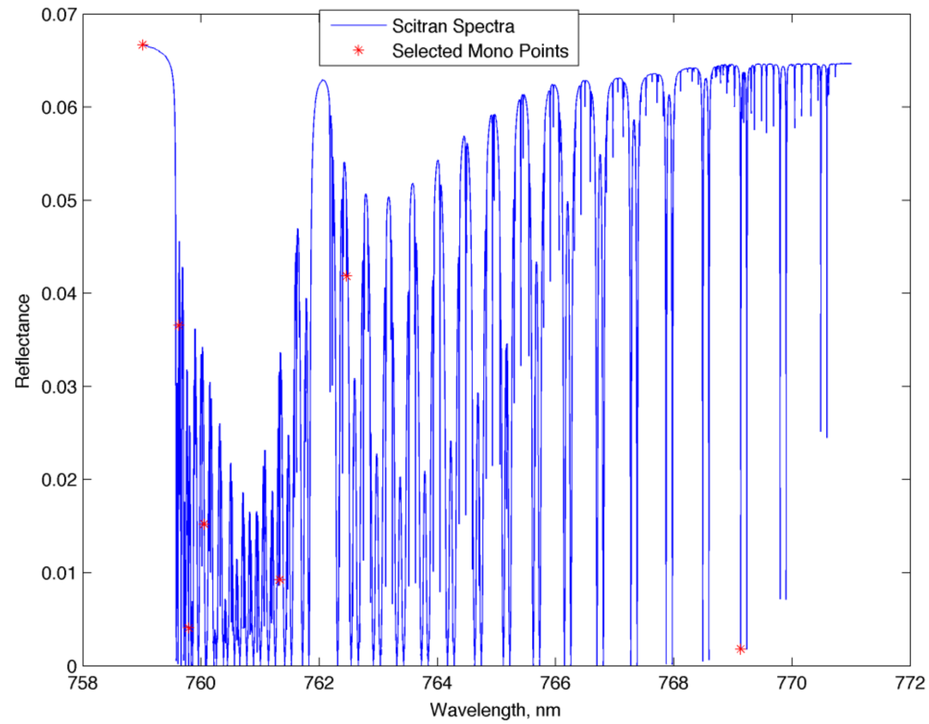


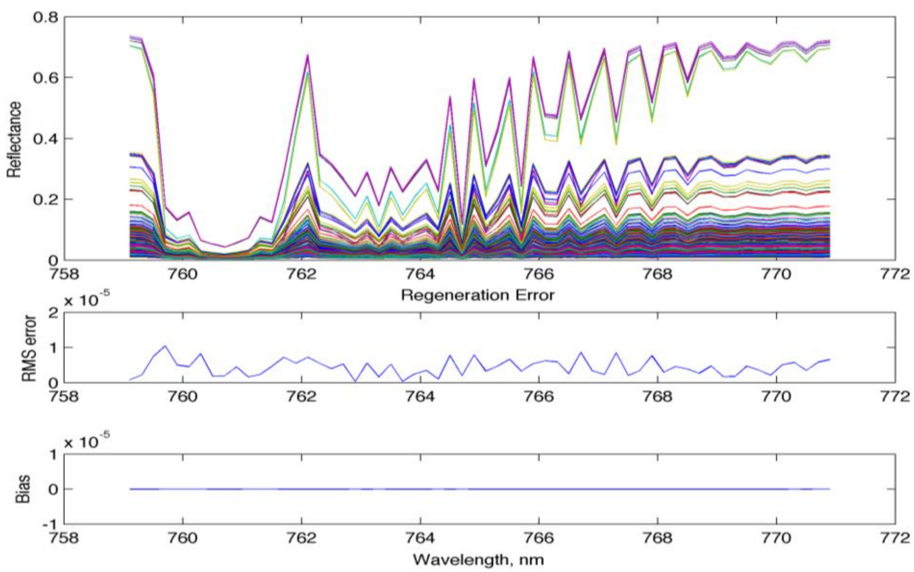




Training PCRTM in Solar (O_2 A-band at OCO and SCIAMACHY spectral resolution)







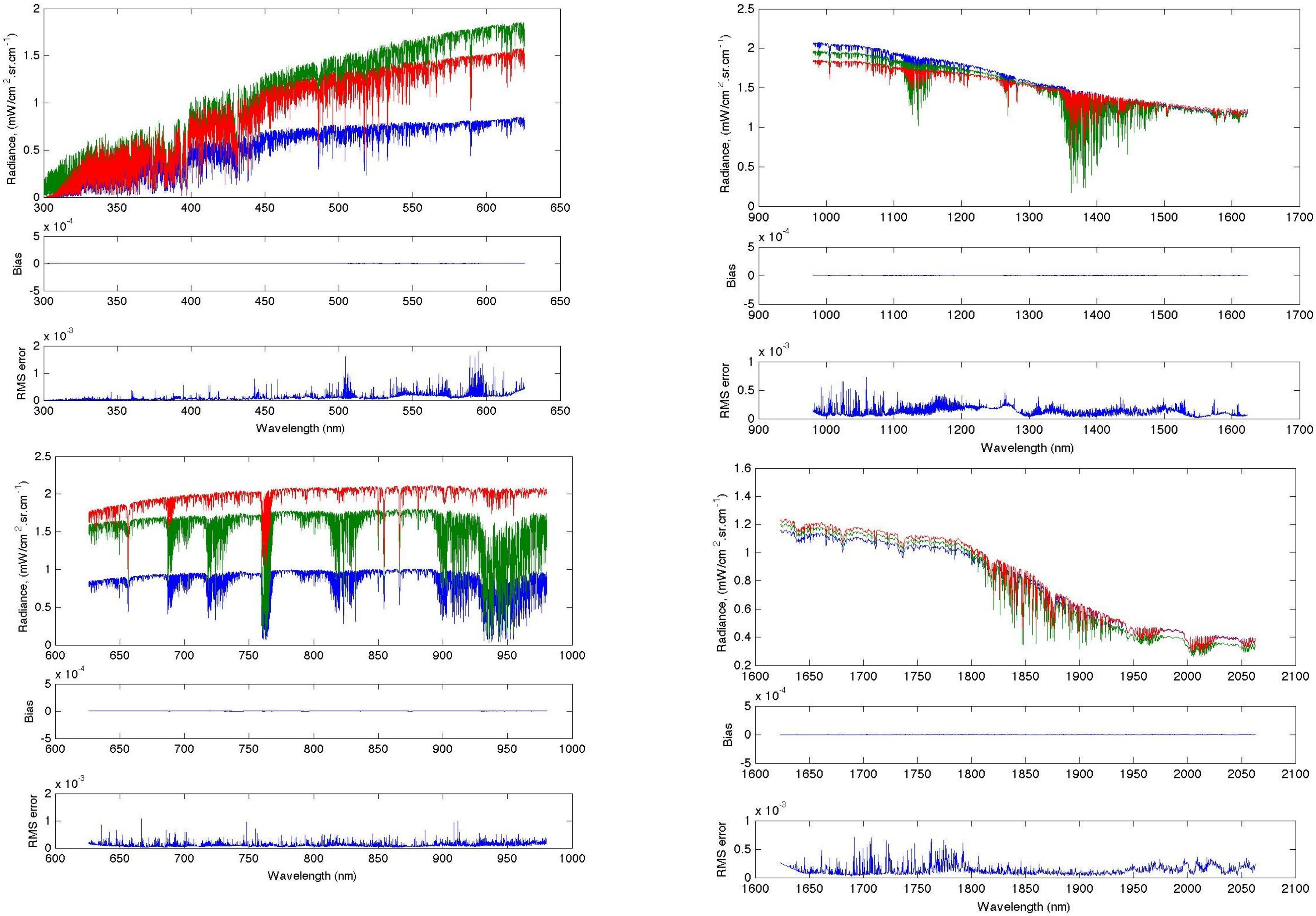
- Model reflectance of R-branch of O_2 A-band
- OCO spectral resolution (0.045 nm)
- 5-6 EOF, 7 Mono needed (out of 12000 from LBL)
- Maximum RMS error < 2.32×10^{-5} for 7500 sample
  - Various clouds
  - Aerosols
  - Ocean and various land surface types
  - Various atmospheric profiles
- Bias error close to zero

Training PCRTM in RS from 0.3 to 2.5 μm

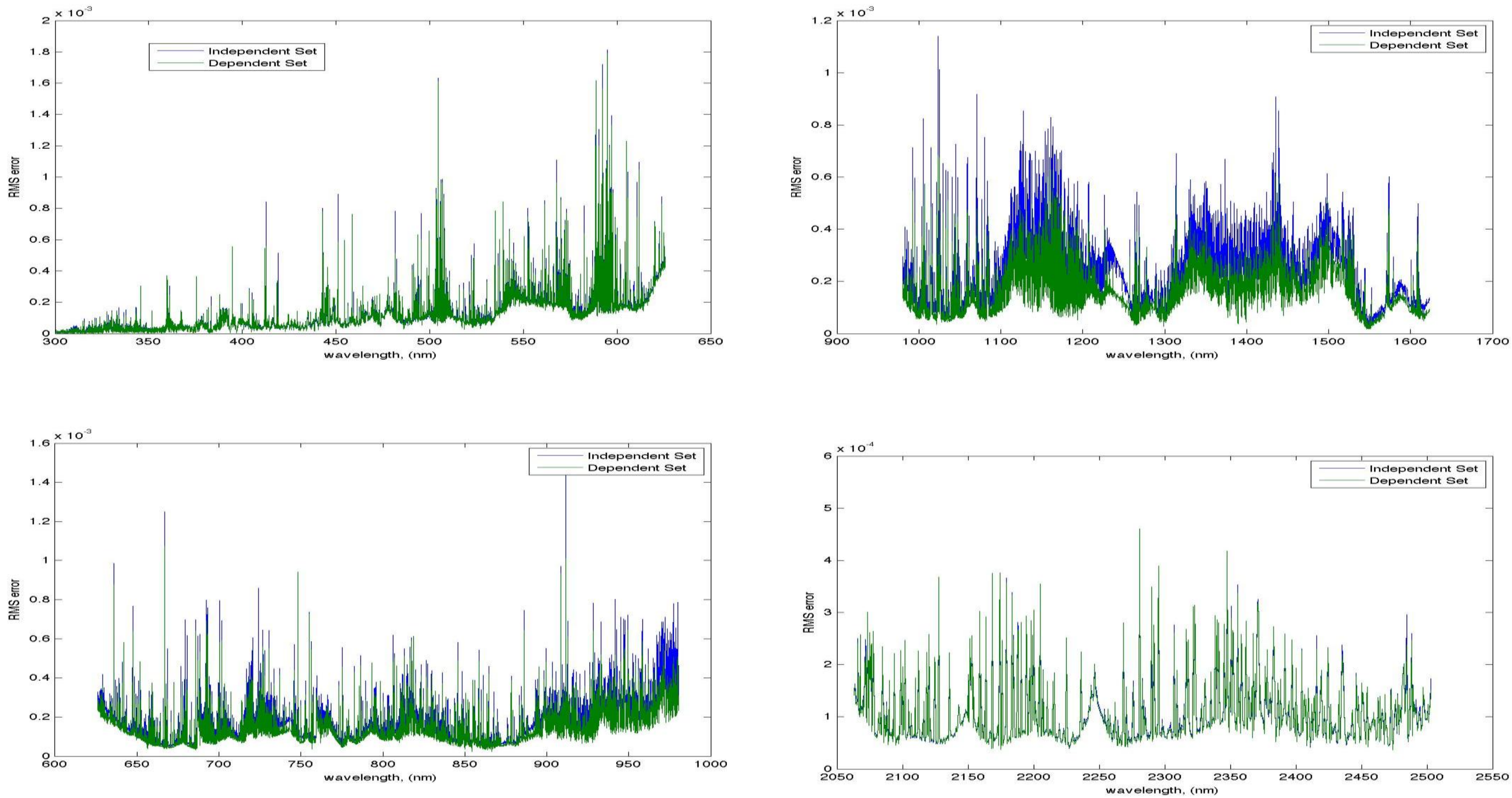
- MODTRAN used as the RT model for training
  - Preliminary training with limited cases
  - Ocean surface only
  - water clouds only
  - 1-17 Ks are used for gas absorptions and the code is modified to output the radiances at each k-node and the weighted-average
  - 12 stream DISORT calculations
- Spectral range: 0.3-2.5 μm with $\Delta v = 1 cm^{-1}$
  - Total of 259029 monochromatic RT performed per spectrum
  - The goal is to reduce the points to 1000-2000
  - Will train PCRTM at 1 cm^{-1} resolution
  - Other spectral resolution can be derived from this high spectral resolution PCRTM
  - Much less mono and PC needed for lower resolution spectra expected
- The following parameters are randomly varied in the MODTRAN runs

Parameter	Range
Solar zenith	0-80°
View zenith	0-70°
Azimuth angle	0-360°
Column water vapor	0.0-6.0 cm
Total column ozone	0-500 Dobson
AOD (Maritime)	0.0-1.0
Wind	3-11 m/s
Cloud τ	0-50
Cloud Ht	1-15 km
Cloud Re	7-28 μm

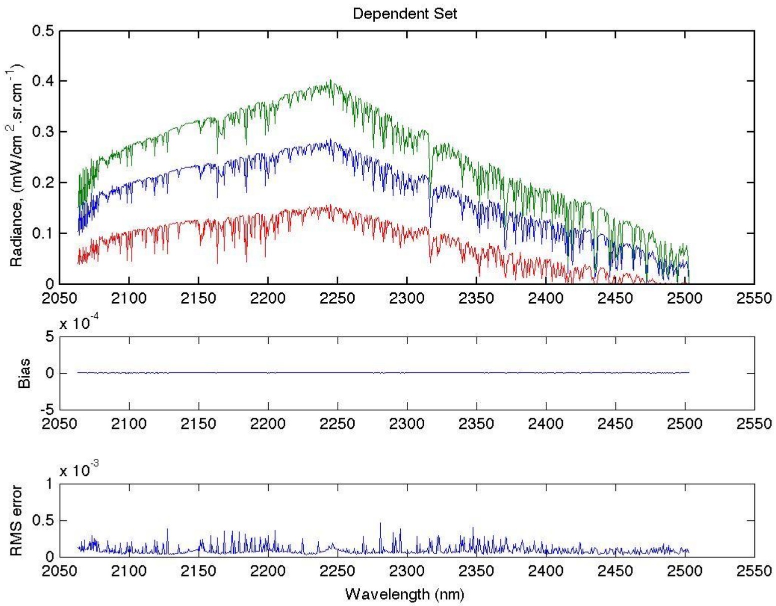
Preliminary results for all spectral regions

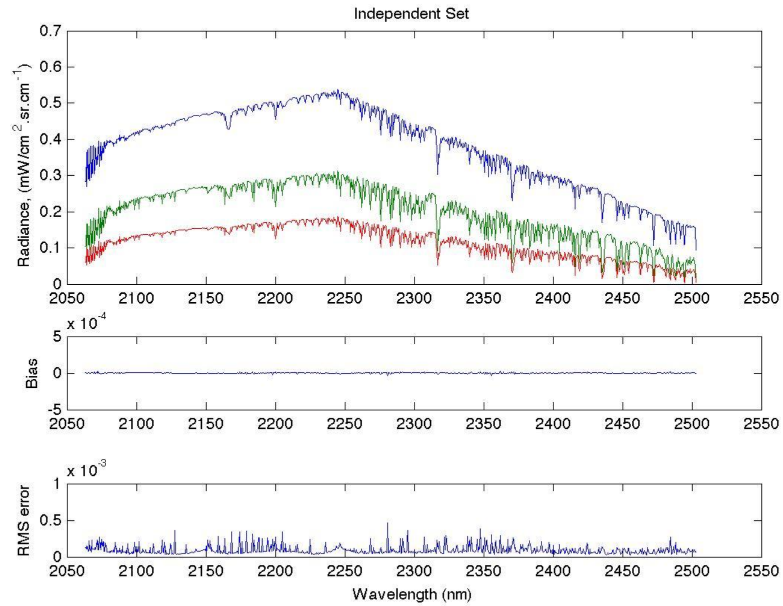


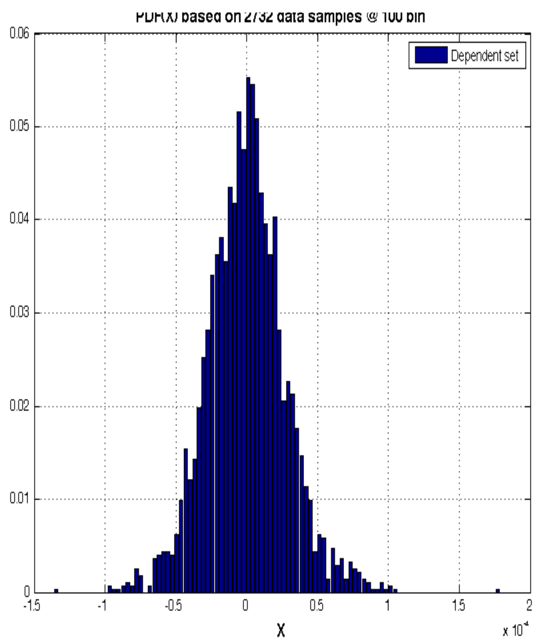
The fitting accuracy has been validated using independent data sets



Preliminary results for all spectral regions (0.3-2.5 μm)







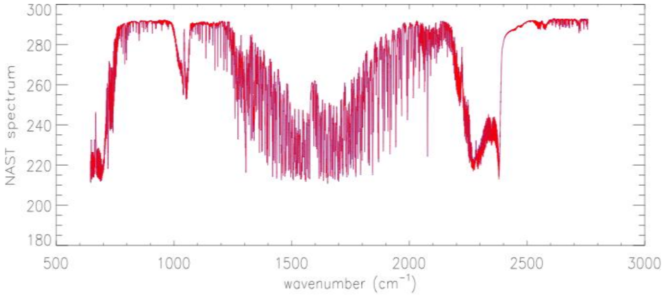
Band No.	Range (μm)	Channel No.	Mono No.	Mono No. (reduced)	EOF No.
1	2.063-2.503	853	14518	84	35
2	1.623-2.062	1313	22372	153	90
3	0.981-1.622	4038	63315	307	265
4	0.626-0.980	5780	82789	172	85
5	0.300-0.625	17327	76226	55	20

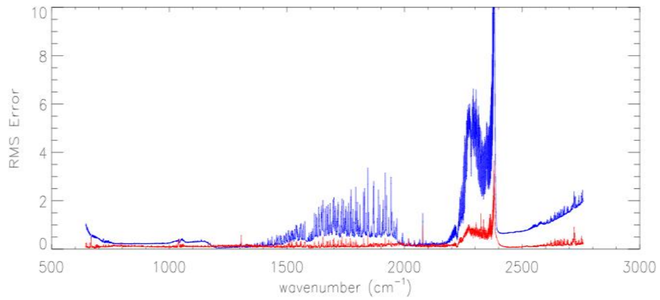
- Current channel number = 23531, need 771 predictors (a factor of 340 less RT computations relative to MODTRAN)
- 4 nm spectral resolution instrument will result in less than 1100 channels (2 nm sampling)
- 300 - 500 mono RT expected for CLARREO type of instrument (520-860 fold speed-up relative to MODTRAN)

Application of PCRTM to real data and to CLARREO studies

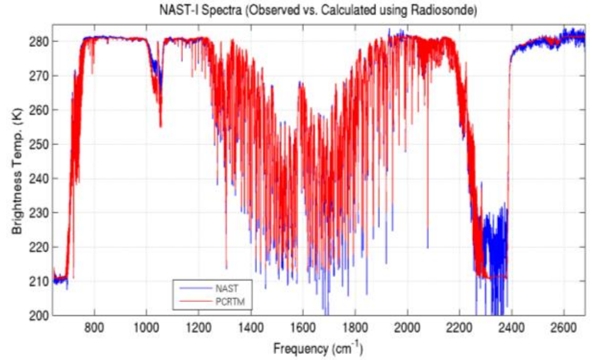
- PCRTM has been validated using real hyperspectral data
  - IASI on Metop satellite
  - NAST-I airborne hyperspectral instrument
  - AIRS on Aqua satellite
  - Both forward model and retrieval applications
- PCRTM has been used for CLARREO studies
  - Orbital data simulations
  - Radiative kernel calculations
  - Instrument trade studies and Information content analysis
  - Filling spectra gaps due to limited instrument spectral range
  - Relating TOA radiance to TOA flux
  - Detecting atmospheric changes using simulated CLARREO data
- PCRTM has been incorporated into a retrieval algorithm based on Optimal Estimation method
  - Retrieval done in EOF space (computationally efficient)
  - T, H_2O, CO_2, CO, O_3, CH_4, N_2O, cloud optical depth, cloud height, cloud phase, cloud particle size, surface emissivity, and surface skin temperature are retrieved simultaneously
  - Retrieval products are consistent with the measurement radiances via PCRTM
  - Been applied to AIRS, NAST-I, and IASI (ready to be applied to CrIS and CLARREO)

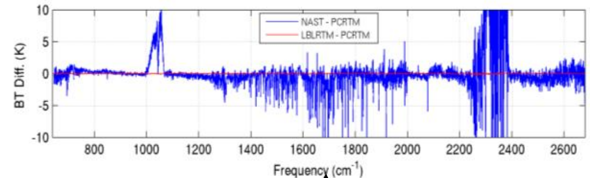
Example PCRTM model has been validated using IASI, NAST-I and AIRS observation data



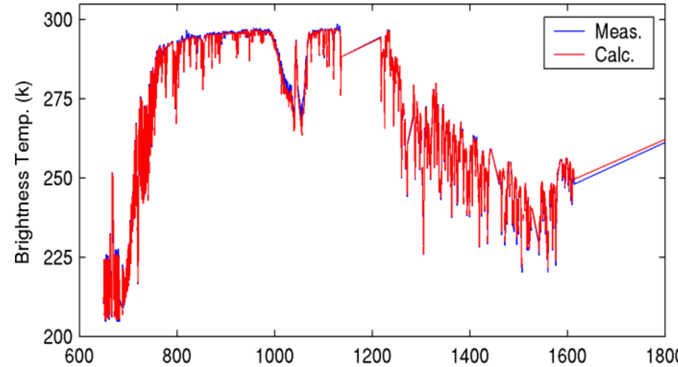


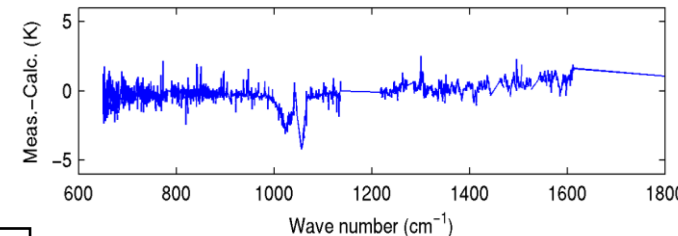
- Comparison of observed and calculated IASI spectra
- Blue line is IASI noise
- Red line is the difference between IASI observation and PCRTM calculations





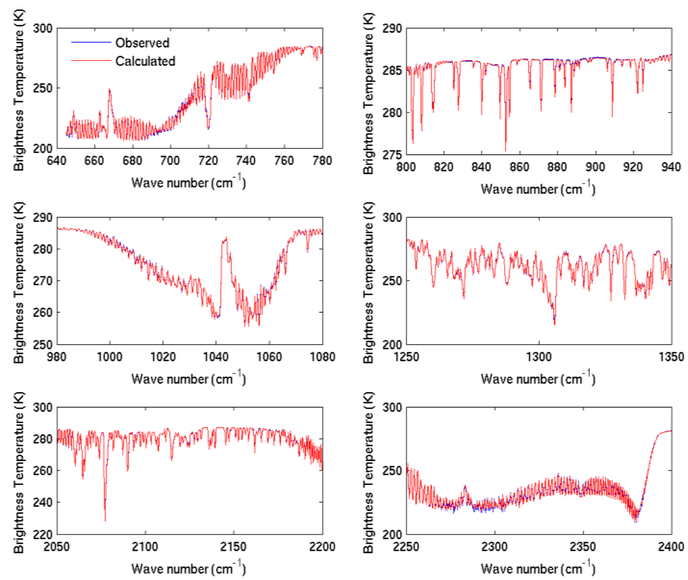
- Observed and calculated NAST-I spectrum





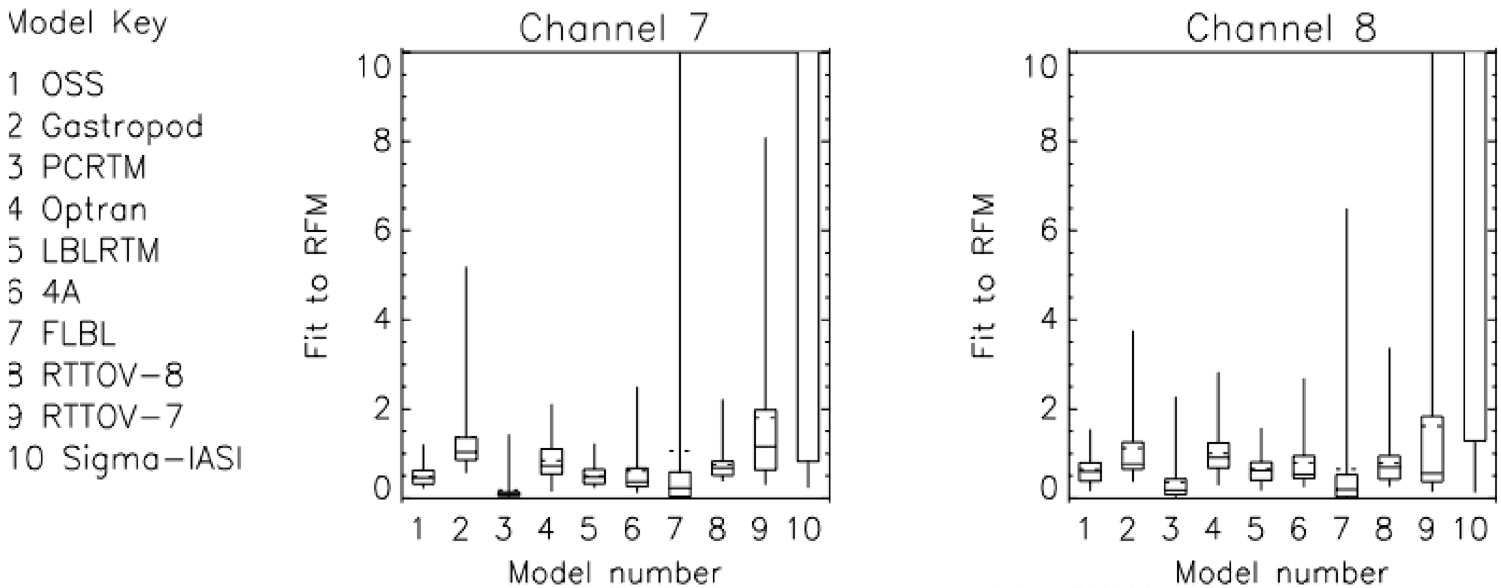
- An example of Observe vs forward model calculated AIRS spectra
- Temperature, H2O and O3 profiles are taking from ECMWF model
- Spikes due to AIRS popping noise not completely removed
- Ozone truth has poor quality

- Expanded plots of observed and PCRTM calculated IASI spectra

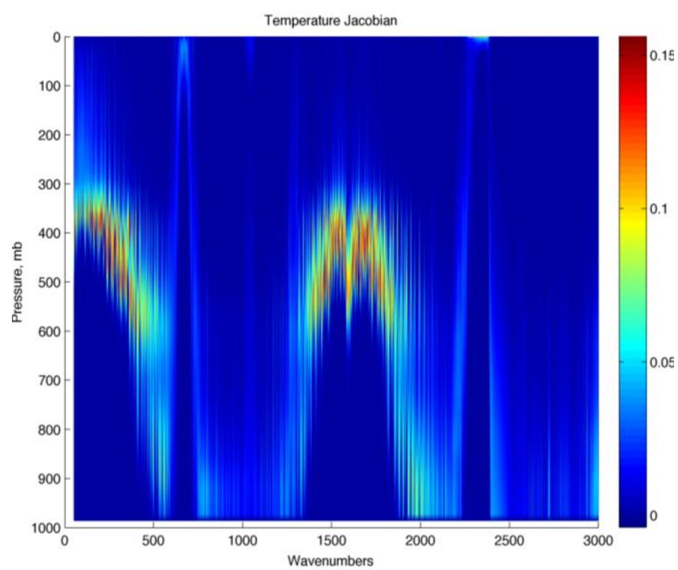


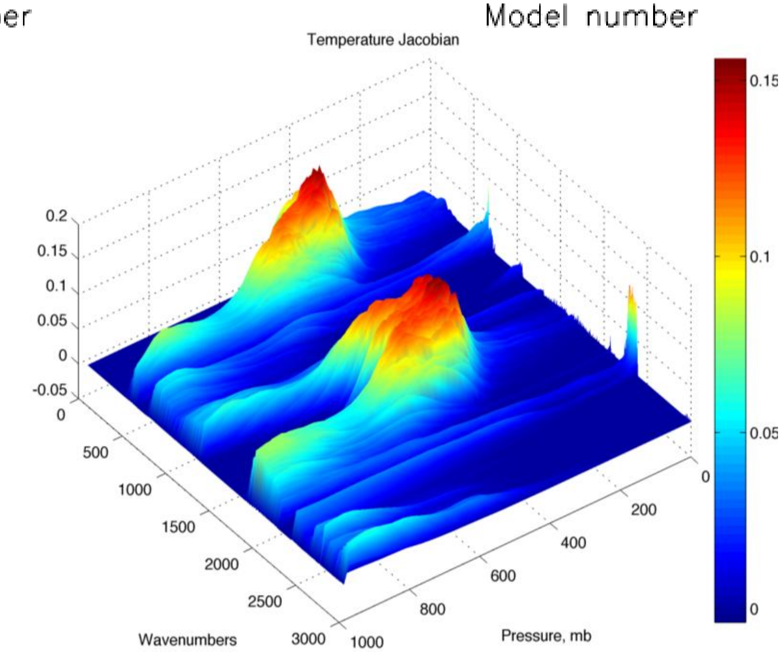
Example of Jacobian from PCRTM

- Comparison of ozone Jacobian from different models (*Saunders et al. JGR, 2006*)



- Temperature Jacobian calculated from PCRTM (see Brian's talk for details)

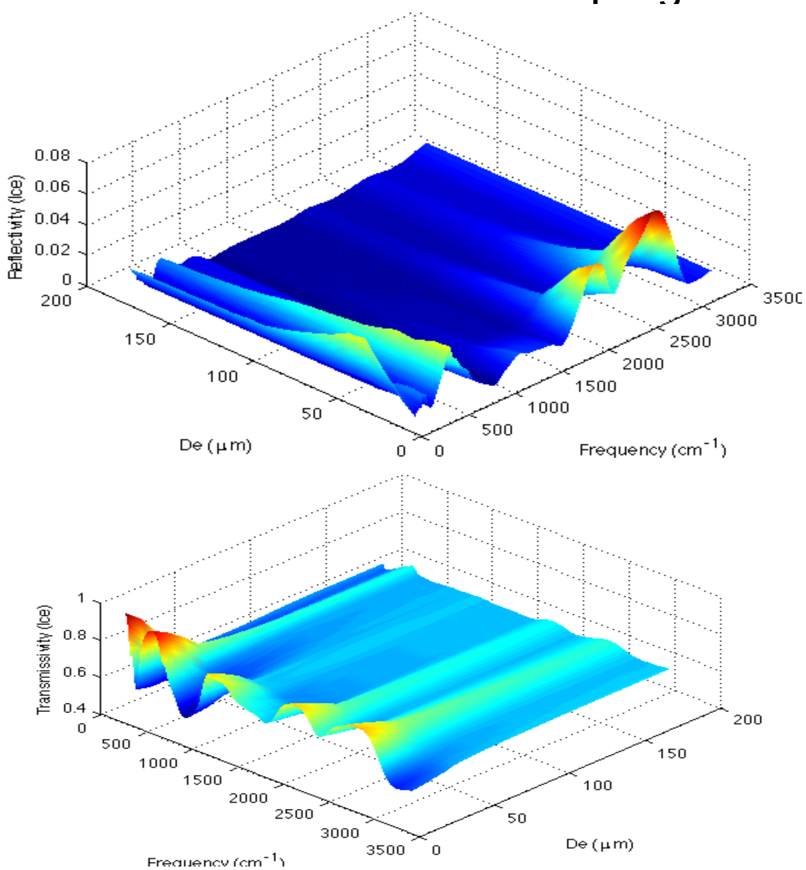


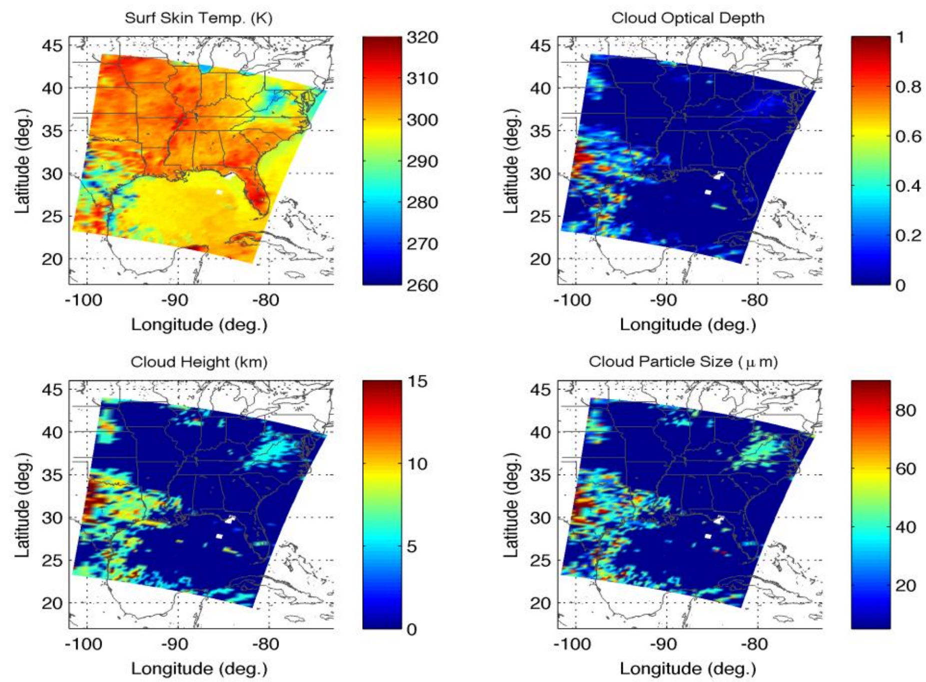


Example of PCRTM cloud modeling and retrieval in thermal infrared spectral region

$$\mu \frac{dR(\tau,\mu)}{d\tau} = R(\tau,\mu) - \frac{1}{2}\omega \int_{-1}^{1} R(\tau,\mu')P(\mu,\mu')d\mu' - \frac{\omega}{4\pi}F_0 P(\mu,-\mu_0)e^{-\tau/\mu_0} + (1-\omega)B[(T(\tau)]$$

- Cloud effective transmissivity and reflectivity calculated using DISORT
  - Dependence on particle size, optical depth, observation angles are captured
  - Orders of magnitude faster compared to running DISORT
- PCRTM retrieved cloud top agrees well with CALIPSO data





Example of predicting the 0-200 cm^{-1} spectral region using CLARREO spectra (200-2000 cm^{-1})

- PCRTM forward model used to predict the missing CLARREO spectral region
  - Fast and easy
- Calculated the mean and error in the mean for integrals for each atmosphere
  - Errors less than 0.026 K
  - Included instrument error
- The simulated measurements are systematically low by a few parts in 1e-3.
  - Due to the random sampling error which affects the responsivity
  - Difference in radiative transfer model (Dave Kratz's LBL model used for truth simulation)

Spectral Range (cm-1)	Integrals from truth (K)	Integral from fitted (K)	Error (K)
0-50	0.0729	0.0680	+/- 0.0006
50-200	2.9814	2.9106	+/- 0.026
200-2000	89.888	89.802	+/- 0.03
0-2000	92.942	92.780	+/- 0.039

Ways to explore information content of CLARREO hyperspectral data

- Invert each instantaneous spectrum first
  - Obtain atmospheric, cloud, and surface properties
  - Study zonal/global mean of the retrieved products
  - Perform time series analysis (taking into account of natural variability)
  - Retrieval done in EOF space

$$X_{n+1} - X_a = (K^T S_y^{-1} K + \lambda I + S_a^{-1})^{-1} K^T S_y^{-1} [(y_n - Y_m) + K(X_n - X_a)]$$

- Perform radiance averaging first
  - Perform retrieval of individual climate variables using spectral fingerprinting method
  - Less sensitive to instantaneous instrument noise
  - All retrieval done in EOF space

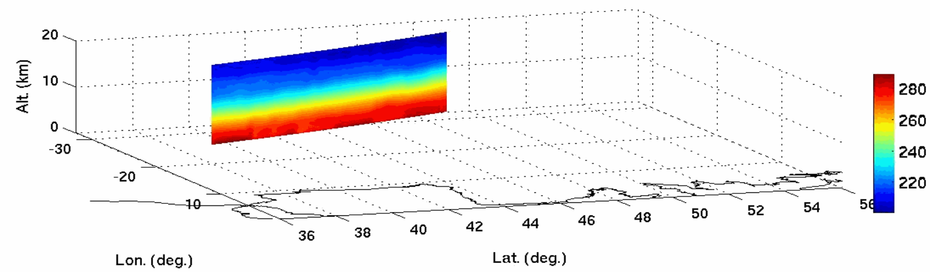
$$y = Kx + e$$

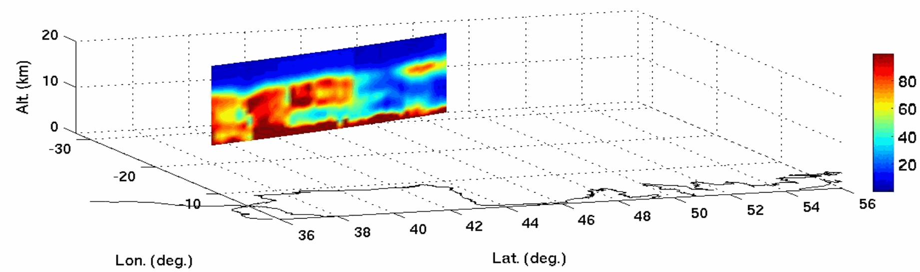
$$a = (K^T S_y{}^{-1} K^{-1} K^T S_y{}^{-1} y$$

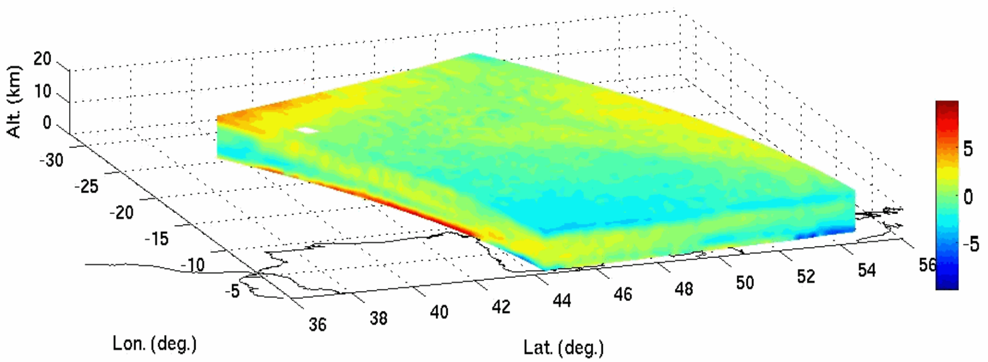
$$S_y = S_{nat} + S_{shape} + S_{nl}$$

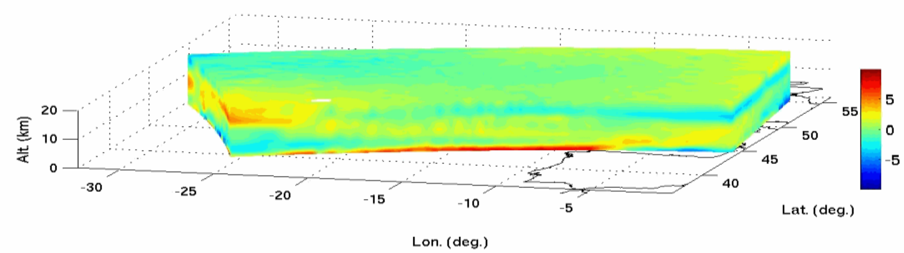
Example of retrieved atmospheric parameters from IASI data

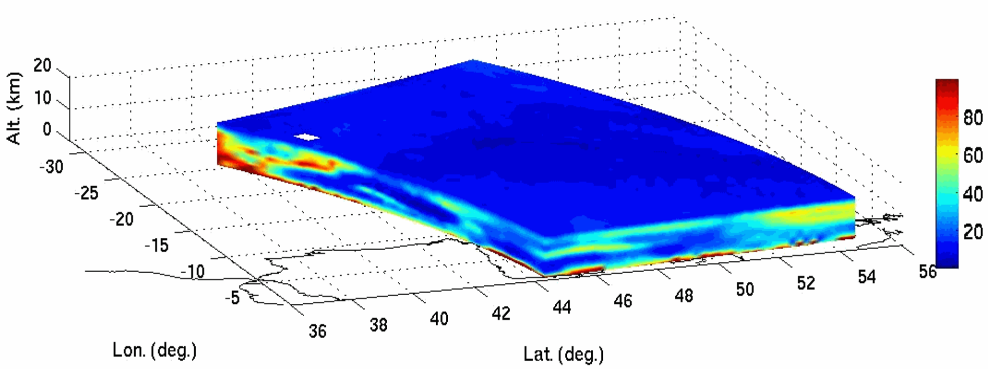
- 3 movies showing IASI temperature and moisture cross-sections on 11/04/2007 over Anglet France
  - T and H_2O as a function of altitude
  - T and H_2O along satellite track
  - T and H_2O x-track
- Note fine atmospheric features capture
- Coherent spatial features

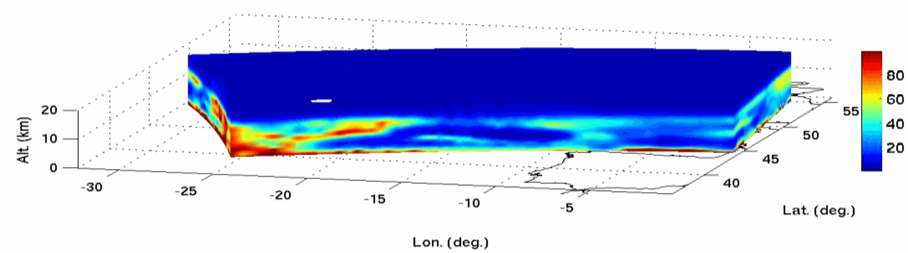




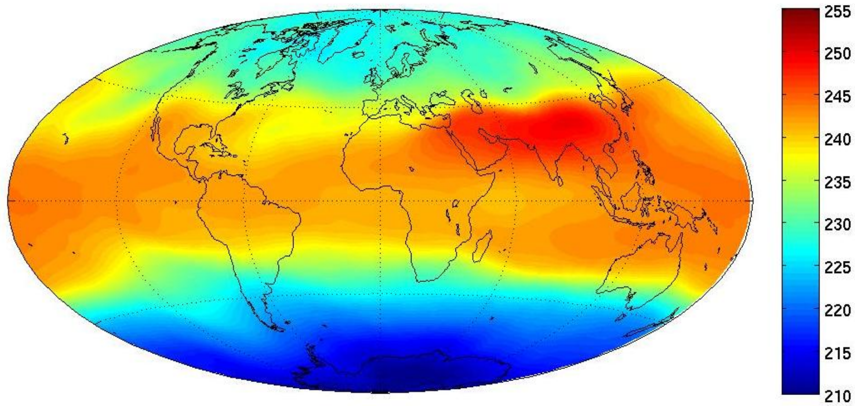


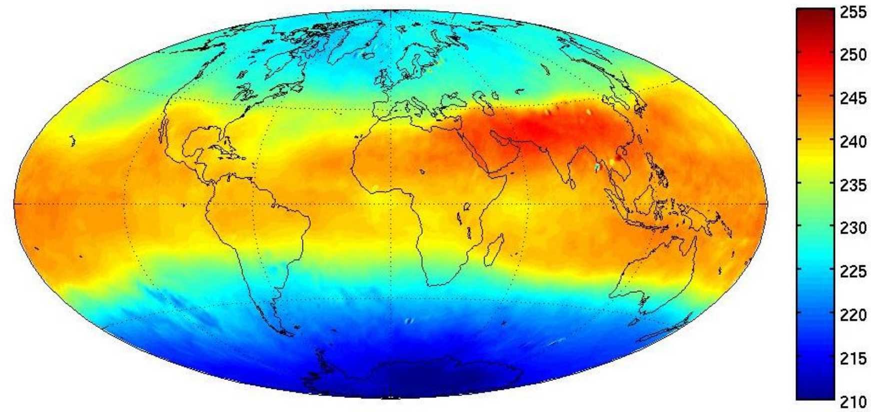


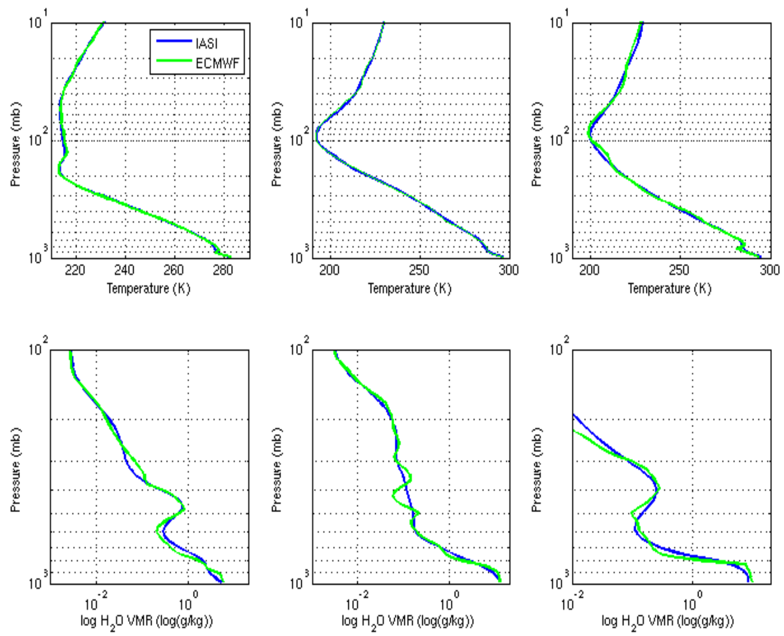




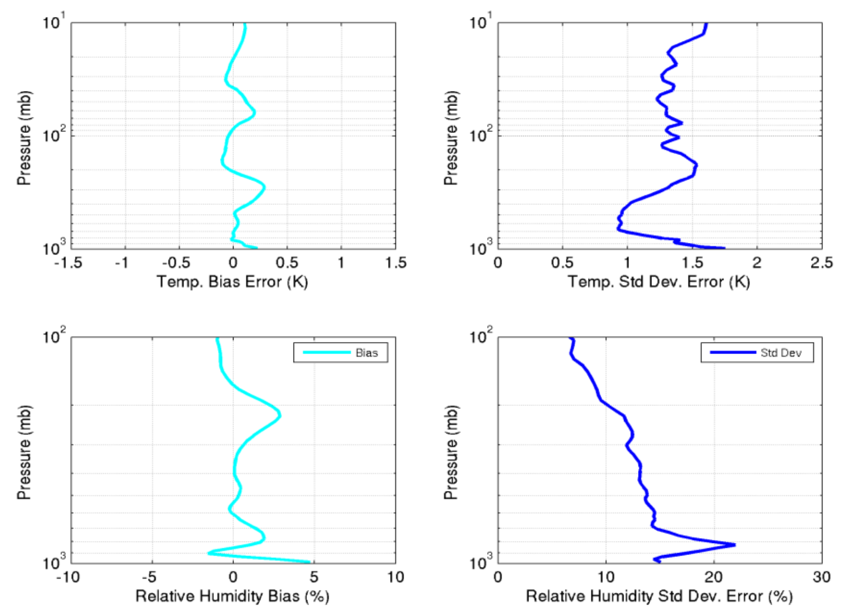
Comparison of PCRTM retrieved temperature and moisture profiles with ECMWF





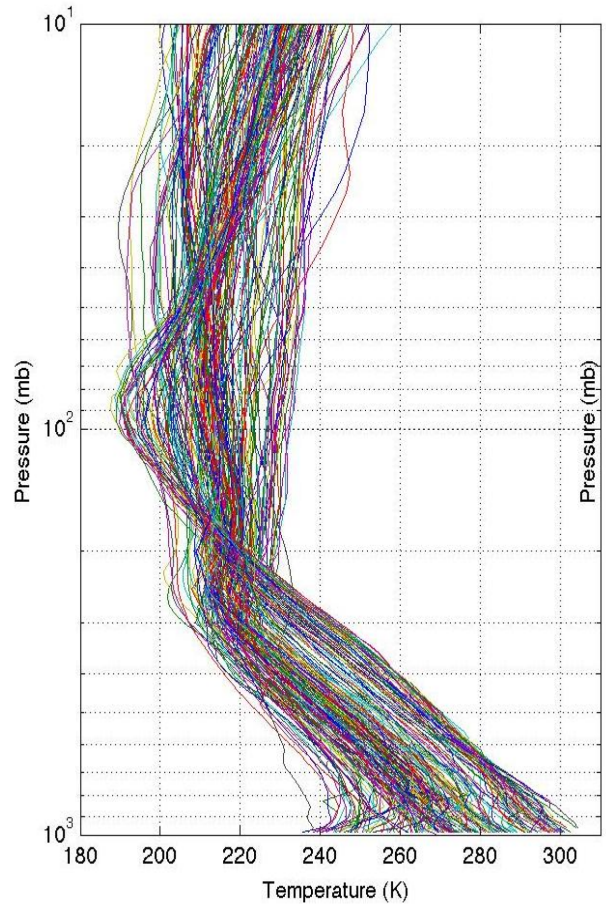


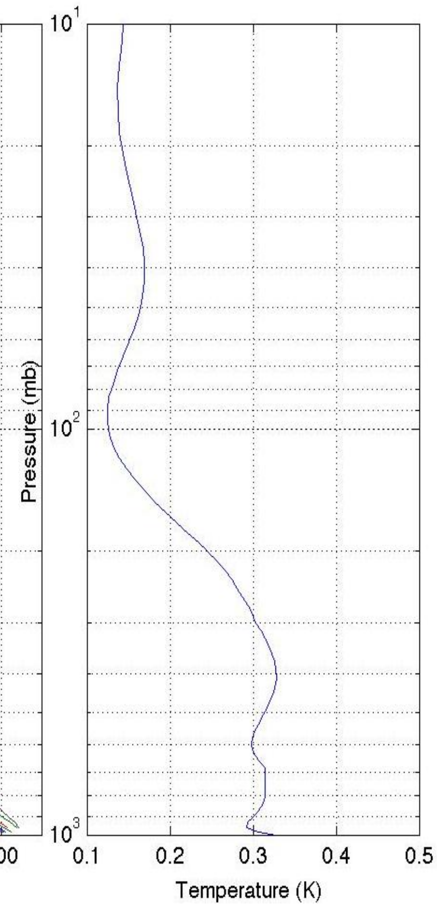
Statistics (101 levels , no vertical averaging)



Simulation/retrieval stud of small atmospheric changes

- 1000 atmospheric profiles selected
- 1000 radiance spectra simulated using PCRTM
- Perturb 1000 atmospheric profiles
  - Perturb temperature by 0.15 K above 200 mb
  - Perturb temperature by 0.31 K below 200 mb
  - Perturb surface skin temperature by 0.27 K
  - Perturb water by 3.16 % above 200 mb
  - Perturb water by 1.63% below 200 mb
- Computes new radiances using perturbed profiles
- Perform retrieval using 2000 spectra
  - Compute atmospheric profile differences
  - Plot the averaged result
- Perform average of the difference spectra
  - Perform optimal fingerprinting using averaged radiance spectrum





Summary and Conclusions

- Forward model is a key component in analysing hyperspectral data
  - End-to-end sensor trade studies
  - Realistic global long term data simulations and OSSE experiment
  - Satellite data analysis and data assimilations
- PCRTM is a useful tool specific for hyperspectral data with thousands of channels
  - PCRTM compresses thousands of spectral channels into few hundred EOFs
  - 3-4 orders of magnitude faster than Line-by-line models
  - 2-100 times faster than traditional forward model
  - Very accurate relative LBL models
  - Multiple scattering cloud calculations included
  - Model has been developed for AIRS, NAST,IASI, CLARREO, and CrIS
  - The method has been extended to UV-VIS-near IR spectral region
- More work needed
  - User-friendly PCRTM code
  - More forward model training in the solar spectral region
  - Continue to explore CLARREO information using both instantaneous and averaged spectra to derive climate related quantities
    - Using simulated spectral from satellite and model products
    - Using IASI as proxy data